Course Type	Course Code	Name of Course	L	T	P	Credit
DE	NPHD502	COMPUTATIONAL PHYSICS	3	0	0	3

Prerequisite: Mathematical Physics, Quantum Mechanics.

Course Objective
• To acquaint the students with highly developed computational methods employed in solving complex problems in physics; • To specialize them for research in theoretical physics in the forefront areas of advanced physical fields.
Learning Outcomes
After attending the course the students will learn about various computational techniques to solve physical problems. They will also be skilled on Monte Carlo and molecular dynamics simulations. Further they will have some useful concepts on parallel computation and MATLAB.

Unit No.	Topics to be Covered	Lecture Hours	Learning Outcome
1	Theory and simulation of in one, two and three dimensions. Elementary ideas and simulations of self-avoiding walks,	4	Student will learn about the modeling and computation of lattice models and its applications in condensed matter physics.
2	Additive and multiplicative stochastic processes, Brownian motion and fractional Brownian motion.	4	The student will learn to deal with physical phenomena with random time evolution such as earthquack and stock market etc.
3	Percolation theory and simulation by Hoshen-Kopelman algorithm; Application to simple lattice models in Physics.	6	The student will learn with the behavior of connected clusters in a random graph describing phase transitions and its applications.
4	Introduction to Hartree-Fock theory and Density functional theory.	4	The student will learn about the DFT and its application in investigating the structural, magnatic and electronic properties of molecules, materials and defects.
5	Computer Simulations: Monte Carlo simulation: Basic idea, Importance Sampling, Metropolis algorithm, Markov chain, and Some applications.	9	At the end of this section of student will learn about the basic methods and tricks of Monte-Carlo simulation. They will also be able to perform MC simulation of simple molecular liquids.
6	Molecular Dynamics: Basic idea, Equation of motion; Program initialization, The force calculation, Integrating the equation of motion and Some applications. Ising model in magnetism, Bak-Tang-Wiesenfeld model in studies of self-organized criticality.	9	At the end of this unit student will learn about the methodology of the simulation of evolving systems. They will also learn about the application of Molecular Dynamic simulation of simple dynamic systems
7	Significance of Parallel Computation in numerical calculation; Introduction to MATLAB Programming with few examples.	6	At the end of this unit student should be able to know the methods and power of Parallel computing. They should be able to write small parallel computer codes.
	Total	**42**	

Text Books:

1. Numerical Recipes: The Art of Scientific Computing; William H. Press; Cambridge University Press; 2007.
2. A Guide to Monte Carlo Simulations in Statistical Physics, D. P. Landau and K. Binder, Cambridge University Press.
3. I. Prigogine and Stuart A. Rice, New Methods in Computational Quantum Mechanics, Wiley.
4. Introduction to Computational Chemistry, Frank Jensen

Reference Books:

1. Matlab: A Practical Introduction to Programming and Problem Solving; Stormy Attaway; Butterworth-Heinemann; 2011.
2. FORTRAN 90 for Scientists and Engineers; Brian Hahn; Butterworth-Heinemann; 1990.
3. Computer Programming in Fortran 77; V. Rajaraman
4. Computational Physics, Joseph Marie Thijssen, Cambridge University Press.
5. An Introduction to Computational Physics, Tao Pang, Cambridge University Press.
6. Computer Simulation of Liquids, M. P. Allen and D. J. Tildesley, Clarendon Press.
7. D. Frankel and B. Smit, Understanding Molecular Simulation, second edition, Academic Press.
8. R. G. Parr and W. Yang, Density Functional theory of atoms and molecules.